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Quantum Computational Geodesics

by Howard E. Brandt

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14. ABSTRACT
Recent developments in the differential geometry of quantum computation offer a new approach to the analysis of quantum computation. In the Riemannian geometry of quantum computation, the quantum evolution is described in terms of the special unitary group of n-qubit unitary operators with unit determinant. The group manifold is taken to be Riemannian. The objective of this report is to mathematically elaborate on characteristics of geodesics describing possible minimal complexity paths in the group manifold representing the unitary evolution associated with a quantum computation. For this purpose the Jacobi equation, generic lifted Jacobi equation, lifted Jacobi equation for varying penalty parameter, and the so-called geodesic derivative are reviewed. These tools are important for investigations of the global characteristics of geodesic paths in the group manifold, and the determination of optimal quantum circuits for carrying out a quantum computation.

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Contents

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1. Objective

The objective of this project is to mathematically investigate characteristics of geodesics, describing possible minimal complexity paths in the group manifold representing the unitary evolution associated with a quantum computation.

2. Approach

In the Riemannian geometry of quantum computation (*1–11*), a Riemannian metric can be chosen on the manifold of the $(4^n - 1)$-dimensional Lie Group $SU(2^n)$ (special unitary group) of n-qubit unitary operators with unit determinant (*1–27*). The traceless Hamiltonian of a quantum computational system is a tangent vector to a point on the group manifold of the n-qubit unitary transformation describing the time evolution of the system. The Hamiltonian H is an element of the Lie algebra $su(2^n)$ of traceless $2^n \times 2^n$ Hermitian matrices (*25–27*) and is tangent at the n-qubit unitary operator U to the evolutionary curve $e^{-iHt}U$ at $t = 0$. (Here and throughout, units are chosen such that Planck's constant divided by 2π is $\hbar = 1$.)

The Riemannian metric (inner product) $\langle ., . \rangle$ is a positive definite bilinear form $\langle H, J \rangle$ defined on tangent vectors (Hamiltonians) H and J. The n-qubit Hamiltonian H can be divided into two parts $P(H)$ and $Q(H)$, where $P(H)$ contains only one and two-body terms, and $Q(H)$ contains more than two-body terms (*1*). Thus,

$$H = P(H) + Q(H), \tag{1}$$

in which P and Q are superoperators acting on H, and obey the following relations:

$$P + Q = I, \quad PQ = QP = 0, \quad P^2 = P, \quad Q^2 = Q, \tag{2}$$

where I is the identity.

The Hamiltonian can be expressed in terms of tensor products of the Pauli matrices. The Pauli matrices are given by (*28*)

$$\begin{aligned}
\sigma_0 &\equiv I \equiv \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_1 \equiv X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \\
\sigma_2 &\equiv Y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 \equiv Z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.
\end{aligned} \tag{3}$$

They are Hermitian,

$$\sigma_i = \sigma_i^\dagger \;, i = 0, 1, 2, 3, \tag{4}$$

where † denotes the adjoint, and, except for σ_0, they are traceless,

$$\mathrm{Tr}\sigma_i = 0, \quad i \neq 0. \tag{5}$$

Their products are given by

$$\sigma_i^2 = I. \tag{6}$$

Also,

$$\sigma_i \sigma_j = i\varepsilon_{ijk}\sigma_k, \quad i, j, k \neq 0, \tag{7}$$

expressed in terms of the totally antisymmetric Levi-Civita symbol with $\varepsilon_{123} = 1$, and using the Einstein sum convention.

An example of equation 1, in the case of a 3-qubit Hamiltonian, is

$$\begin{aligned} P(H) = x_1\sigma_1 \otimes I \otimes I \quad & + x_2\sigma_2 \otimes I \otimes I + x_3\sigma_3 \otimes I \otimes I \\ & + x_4 I \otimes \sigma_1 \otimes I + x_5 I \otimes \sigma_2 \otimes I + x_6 I \otimes \sigma_3 \otimes I + x_7 I \otimes I \otimes \sigma_1 \\ & + x_8 I \otimes I \otimes \sigma_2 + x_9 I \otimes I \otimes \sigma_3 + x_{10}\sigma_1 \otimes \sigma_2 \otimes I + x_{11}\sigma_1 \otimes I \otimes \sigma_2 \\ & + x_{12} I \otimes \sigma_1 \otimes \sigma_2 + x_{13}\sigma_2 \otimes \sigma_1 \otimes I + x_{14}\sigma_2 \otimes I \otimes \sigma_1 + x_{15} I \otimes \sigma_2 \otimes \sigma_1 \\ & + x_{16}\sigma_1 \otimes \sigma_3 \otimes I + x_{17}\sigma_1 \otimes I \otimes \sigma_3 + x_{18} I \otimes \sigma_1 \otimes \sigma_3 + x_{19}\sigma_3 \otimes \sigma_1 \otimes I \\ & + x_{20}\sigma_3 \otimes I \otimes \sigma_1 + x_{21} I \otimes \sigma_3 \otimes \sigma_1 + x_{22}\sigma_2 \otimes \sigma_3 \otimes I + x_{23}\sigma_2 \otimes I \otimes \sigma_3 \\ & + x_{24} I \otimes \sigma_2 \otimes \sigma_3 + x_{25}\sigma_3 \otimes \sigma_2 \otimes I + x_{26}\sigma_3 \otimes I \otimes \sigma_2 + x_{27} I \otimes \sigma_3 \otimes \sigma_2 \\ & + x_{28}\sigma_1 \otimes \sigma_1 \otimes I + x_{29}\sigma_2 \otimes \sigma_2 \otimes I + x_{30}\sigma_3 \otimes \sigma_3 \otimes I + x_{31}\sigma_1 \otimes I \otimes \sigma_1 \\ & + x_{32}\sigma_2 \otimes I \otimes \sigma_2 + x_{33}\sigma_3 \otimes I \otimes \sigma_3 + x_{34} I \otimes \sigma_1 \otimes \sigma_1 + x_{35} I \otimes \sigma_2 \otimes \sigma_2 \\ & + x_{36} I \otimes \sigma_3 \otimes \sigma_3, \end{aligned} \tag{8}$$

in which ⊗ denotes the tensor product, and

$$\begin{aligned} Q(H) \quad = \quad & x_{37}\sigma_1 \otimes \sigma_2 \otimes \sigma_3 + x_{38}\sigma_1 \otimes \sigma_3 \otimes \sigma_2 \\ & + x_{39}\sigma_2 \otimes \sigma_1 \otimes \sigma_3 + x_{40}\sigma_2 \otimes \sigma_3 \otimes \sigma_1 \qquad (9) \\ & + x_{41}\sigma_3 \otimes \sigma_1 \otimes \sigma_2 + x_{42}\sigma_3 \otimes \sigma_2 \otimes \sigma_1 \\ & + x_{43}\sigma_1 \otimes \sigma_1 \otimes \sigma_2 + x_{44}\sigma_1 \otimes \sigma_2 \otimes \sigma_1 \\ & + x_{45}\sigma_2 \otimes \sigma_1 \otimes \sigma_1 + x_{46}\sigma_1 \otimes \sigma_1 \otimes \sigma_3 \\ & + x_{47}\sigma_1 \otimes \sigma_3 \otimes \sigma_1 + x_{48}\sigma_3 \otimes \sigma_1 \otimes \sigma_1 \\ & + x_{49}\sigma_2 \otimes \sigma_2 \otimes \sigma_1 + x_{50}\sigma_2 \otimes \sigma_1 \otimes \sigma_2 \\ & + x_{51}\sigma_1 \otimes \sigma_2 \otimes \sigma_2 + x_{52}\sigma_2 \otimes \sigma_2 \otimes \sigma_3 \\ & + x_{53}\sigma_2 \otimes \sigma_3 \otimes \sigma_2 + x_{54}\sigma_3 \otimes \sigma_2 \otimes \sigma_2 \\ & + x_{55}\sigma_3 \otimes \sigma_3 \otimes \sigma_1 + x_{56}\sigma_3 \otimes \sigma_1 \otimes \sigma_3 \\ & + x_{57}\sigma_1 \otimes \sigma_3 \otimes \sigma_3 + x_{58}\sigma_3 \otimes \sigma_3 \otimes \sigma_2 \\ & + x_{59}\sigma_3 \otimes \sigma_2 \otimes \sigma_3 + x_{60}\sigma_2 \otimes \sigma_3 \otimes \sigma_3 \\ & + x_{61}\sigma_1 \otimes \sigma_1 \otimes \sigma_1 + x_{62}\sigma_2 \otimes \sigma_2 \otimes \sigma_2 \\ & + x_{63}\sigma_3 \otimes \sigma_3 \otimes \sigma_3. \end{aligned} \tag{10}$$

Here, all possible tensor products of one and two-qubit Pauli matrix operators on three qubits appear in $P(H)$, and analogously, all possible tensor products of three-qubit operators appear in $Q(H)$. Tensor products including only the identity are excluded because the Hamiltonian is taken to be traceless. Each of the terms in equations 8 and 9 is an 8×8 matrix. The various tensor products of Pauli matrices such as those appearing in equations 8 and 9 are referred to as generalized Pauli matrices. In the case of an n-qubit Hamiltonian, there are $4^n - 1$ possible tensor products (corresponding to the dimension of $SU(2^n)$), and each term is a 2^nx2^n matrix.

The right-invariant (*16–18, 26, 27*) Riemannian metric for tangent vectors H and J is given by (*1*)

$$\langle H, J\rangle \equiv \frac{1}{2^n}\mathrm{Tr}\left[HP(J) + qHQ(J)\right]. \tag{11}$$

Here q is a large penalty parameter that taxes more than two-body terms. The length l of an evolutionary path on the $SU(2^n)$ manifold is given by the integral over time t from an initial time t_i to a final time t_f, namely,

$$l = \int_{t_i}^{t_f} dt\left(\langle H(t), H(t)\rangle\right)^{1/2}, \tag{12}$$

and is a measure of the cost, in terms of quantum circuit complexity, of applying a control Hamiltonian $H(t)$ along the path (*1*).

In order to obtain the Levi-Civita connection on the group manifold, one exploits the Lie algebra $su(2^n)$ associated with the group $SU(2^n)$. Because of the right-invariance of the metric, if the connection is calculated at the origin, the same expression applies everywhere on the manifold. Following reference 1, consider the unitary transformation

$$U = e^{-iX} \tag{13}$$

in the neighborhood of the identity $I \subset SU(2^n)$ with

$$X = x\cdot\sigma \equiv \sum_\sigma x_\sigma \sigma. \tag{14}$$

Equation 14 expresses symbolically terms like those in equations 8 and 9 generalized to 2^n dimensions. In equations 12 and 13, X is defined in terms of U using the standard branch of the logarithm with a cut along the negative real axis. In equation 13, for the general case of n qubits, x represents the set of real $(4^n - 1)$ coefficients of the generalized Pauli matrices σ, which represent all of the n-fold tensor products. Taking the trace of equation 13, it follows that the factor x^σ multiplying a particular term σ is given by

$$x^\sigma = \frac{1}{2^n}\mathrm{Tr}(X\sigma). \tag{15}$$

The right-invariant metric, equation 10, can be written as

$$\langle H, J\rangle = \frac{1}{2^n}\mathrm{Tr}[HG(J)], \tag{16}$$

in which the positive self-adjoint superoperator G is given by

$$G = P + qQ. \tag{17}$$

Using equations 2 and 16, it follows that

$$F \equiv G^{-1} = P + q^{-1}Q. \tag{18}$$

A vector Y in the group tangent space can be written as

$$Y = \sum_{\sigma} y^{\sigma}\sigma \tag{19}$$

with so-called Pauli coordinates y^{σ}. Here σ, as an index, is used to refer to a particular tensor product appearing in the generalized Pauli matrix σ. This index notation, used throughout, is a convenient abbreviation for the actual numerical indices (e.g., in equation 9, the number 57 appearing in x_{57}, the coefficient of $\sigma_1 \otimes \sigma_3 \otimes \sigma_3$).

Next consider a curve passing through the origin with tangent vector Y having components $y^{\sigma} = dx^{\sigma}/dt$. It can be shown that the covariant derivative of a right-invariant vector field Z along the curve in the Hamiltonian representation is given by (*1, 2*)

$$(\nabla_Y Z) = \frac{i}{2}\{[Y, Z] + F([Y, G(Z)] + [Z, G(Y)])\}. \tag{20}$$

Because of the right-invariance of the metric, equation 19 is true everywhere on the manifold.

The Riemann curvature on the group manifold affects the behavior of geodesics and can be obtained as follows. In the case of a right-invariant vector field Z, one has after substituting

$$Z = \sum_{\tau} z^{\tau}\tau, \quad Y = \sum_{\sigma} y^{\sigma}\sigma \tag{21}$$

in equation 20,

$$\nabla_{\sigma}\tau = \frac{i}{2}\left([\sigma, \tau] + F([\sigma, G(\tau)] + [\tau, G(\sigma)])\right). \tag{22}$$

Next denote S_0 as a set containing only tensor products of the identity, and S_{12} as the set of terms in the Hamiltonian containing only one and two body terms, that is

$$S_0 \equiv \{I \otimes I \otimes ...\}, \tag{23}$$

and

$$S_{12} = \{I \otimes I \otimes ...\sigma_i \otimes I..,..\} \\ \cup\{I \otimes I \otimes ...\sigma_i \otimes I..\sigma_j \otimes I..,..\}. \tag{24}$$

Evidently then

$$[\sigma, G(\tau)] = \begin{cases} [\sigma,\tau], & \tau \in S_{12} \cup S_0 \\ q[\sigma,\tau], & \tau \notin S_{12} \cup S_0 \end{cases}, \tag{25}$$

and therefore

$$F\left([\sigma, G(\tau)]\right) = \begin{cases} F([\sigma,\tau]), & \tau \in S_{12} \cup S_0 \\ qF([\sigma,\tau]), & \tau \notin S_{12} \cup S_0 \end{cases}. \tag{26}$$

Using equation 18 in equation 26, one obtains

$$F\left([\sigma, G(\tau)]\right) = \begin{cases} \frac{1}{q_{[\sigma,\tau]}}[\sigma,\tau], & \tau \in S_{12} \cup S_0 \\ \frac{q}{q_{[\sigma,\tau]}}[\sigma,\tau], & \tau \notin S_{12} \cup S_0 \end{cases}, \tag{27}$$

where

$$q_{[\sigma,\tau]} = 1 \text{ if } [\sigma,\tau] = 0, \quad q_{[\sigma,\tau]} = q_\lambda \text{ if } [\sigma,\tau] \propto \lambda, \text{ and } q_{[\sigma,\tau]} = q_{[\tau,\sigma]}, \tag{28}$$

and q_λ is defined by

$$q_\sigma \equiv \begin{cases} 0, & \sigma \in S_0 \\ 1, & \sigma \in S_{12} \\ q, & \sigma \notin S_0 \cup S_{12} \end{cases}. \tag{29}$$

Equation 27 can also be written as

$$F\left([\sigma, G(\tau)]\right) = \frac{q_\tau}{q_{[\sigma,\tau]}}[\sigma,\tau]. \tag{30}$$

Next substituting equation 30 in equation 22, and using equation 28, one obtains

$$\nabla_\sigma \tau = i c_{\sigma,\tau}[\sigma,\tau], \tag{31}$$

where

$$c_{\sigma,\tau} = \frac{1}{2}\left(1 + \frac{q_\tau - q_\sigma}{q_{[\sigma,\tau]}}\right). \tag{32}$$

The Riemann curvature tensor with the inner-product (metric) equation 16 is given by (*29*)

$$R(W,X,Y,Z) = \left\langle \nabla_W \nabla_X Y - \nabla_X \nabla_W Y - \nabla_{i[W,X]} Y, Z \right\rangle. \tag{33}$$

After substituting the vector fields,

$$W = \sum_\sigma w^\rho \rho, \quad X = \sum_\sigma z^\sigma \sigma, \quad Y = \sum_\tau y^\tau \tau, \quad Z = \sum_\mu z^\mu \mu, \tag{34}$$

equation 33 becomes

$$R_{\rho\sigma\tau\mu} = \left\langle \nabla_\rho \nabla_\sigma \tau - \nabla_\sigma \nabla_\rho \tau - \nabla_{i[\rho,\sigma]}\tau, \mu \right\rangle. \tag{35}$$

Next, for three right-invariant vector fields X, Y, and Z, one has

$$0 = \nabla_Y \langle X, Z \rangle = \langle X, \nabla_Y Z \rangle + \langle \nabla_Y X, Z \rangle , \tag{36}$$

or

$$\langle X, \nabla_Y Z \rangle = - \langle \nabla_Y X, Z \rangle , \tag{37}$$

and substituting equation 34 in equation 37, one then has

$$\langle \sigma, \nabla_\tau \mu \rangle = - \langle \nabla_\tau \sigma, \mu \rangle . \tag{38}$$

Then replacing the vector σ in equation 38 by the vector $\nabla_\sigma \tau$, equation 31 (see equation 7), one has

$$\langle \nabla_\rho \nabla_\sigma \tau, \mu \rangle = - \langle \nabla_\sigma \tau, \nabla_\rho \mu \rangle , \tag{39}$$

and interchanging indices ρ and σ, then

$$\langle \nabla_\sigma \nabla_\rho \tau, \mu \rangle = - \langle \nabla_\rho \tau, \nabla_\sigma \mu \rangle . \tag{40}$$

Then substituting equations 39 and 40 in equation 35, and interchanging the first and second terms, one obtains

$$R_{\rho\sigma\tau\mu} = \langle \nabla_\rho \tau, \nabla_\sigma \mu \rangle - \langle \nabla_\sigma \tau, \nabla_\rho \mu \rangle - \left\langle \nabla_{i[\rho,\sigma]} \tau, \mu \right\rangle . \tag{41}$$

Also clearly

$$\nabla_{iY} Z = i \nabla_Y Z, \tag{42}$$

so equation 41 can also be written as

$$R_{\rho\sigma\tau\mu} = \langle \nabla_\rho \tau, \nabla_\sigma \mu \rangle - \langle \nabla_\sigma \tau, \nabla_\rho \mu \rangle - i \left\langle \nabla_{[\rho,\sigma]} \tau, \mu \right\rangle . \tag{43}$$

Next substituting equation 31 in equation 43, one obtains the following useful form for the Riemann curvature tensor (*1*):

$$\begin{aligned} R_{\rho\sigma\tau\mu} &= c_{\rho,\tau} c_{\sigma,\mu} \langle i[\rho,\tau], i[\sigma,\mu] \rangle \\ &\quad - c_{\sigma,\tau} c_{\rho,\mu} \langle i[\sigma,\tau], i[\rho,\mu] \rangle \\ &\quad - c_{[\rho,\sigma],\tau} \langle i[i[\rho,\sigma],\tau], \mu \rangle . \end{aligned} \tag{44}$$

The geodesic equation on the $SU(2^n)$ group manifold with the Riemannian metric, equation 16, is obtained as follows. Consider a curve passing through the origin with tangent vector Y having components $y^\sigma = dx^\sigma/dt$. The covariant derivative along the curve in the Hamiltonian representation is given by (*1, 2*)

$$(D_t Z) \equiv (\nabla_Y Z) = \frac{dZ}{dt} + \frac{i}{2} \left([Y, Z] + F \left([Y, G(Z)] + [Z, G(Y)] \right) \right) . \tag{45}$$

(Note that the term $\frac{dZ}{dt}$ in equation 45 does not appear in equation 20 because there the vector field Z is taken to be right invariant, in which case $\frac{dZ}{dt} = 0$.). Equation 45 is true on

the entire manifold because of the right-invariance of the metric. Furthermore, a geodesic in the $SU(2^n)$ manifold is a curve $U(t)$ with tangent vector $H(t)$ parallel transported along the curve, namely,

$$D_t H = 0. \tag{46}$$

However, according to equation 45 with $Y = Z = H$, one has

$$D_t H = \frac{dH}{dt} + \frac{i}{2}([H, H] + F([H, G(H)] + [H, G(H)])), \tag{47}$$

which when substituting equation 46 becomes (*1*)

$$\frac{dH}{dt} = -iF([H, G(H)]). \tag{48}$$

One can rewrite equation 48 using the dual L of H (*1, 2*) and equation 18,

$$L \equiv G(H) = F^{-1}(H), \tag{49}$$

and then noting that

$$\frac{dL}{dt} = \frac{d}{dt}\left(F^{-1}(H)\right) = F^{-1}\left(\frac{dH}{dt}\right). \tag{50}$$

Thus substituting equation 48 in equation 50, one obtains

$$\frac{dL}{dt} = -iF^{-1}(F([H, G(H)])), \tag{51}$$

or

$$\frac{dL}{dt} = -i[H, G(H)], \tag{52}$$

and again using equations 50 and 52 it becomes

$$\frac{dL}{dt} = -i[H, L] = i[L, H]. \tag{53}$$

Furthermore, again using equation 50 in equation 53, one obtains the sought geodesic equation (*1*):

$$\frac{dL}{dt} = i[L, F(L)]. \tag{54}$$

This equation is a Lax equation, a well-known nonlinear differential matrix equation, and L and $iF(L)$ are Lax pairs (*30–32*). Some solutions to the geodesic equation, equation 54, are given in references 1 and 7.

3. Results

Jacobi fields describe the divergence or convergence of neighboring geodesics and are useful in determining conjugate points. Conjugate points are points on a geodesic at which the Jacobi field is vanishing without vanishing in between these points. It is well-known that past the first conjugate point, a geodesic ceases to be minimizing (*15, 18*). Jacobi fields are first to be addressed here for a general Riemannian manifold. Following this, Jacobi fields will be specialized to the $SU(2^n)$ group manifold germane to quantum computation.

Consider a one-parameter family of geodesics on a generic Riemannian manifold,

$$x^j = x^j(s,t), \tag{55}$$

in which the parameter s distinguishes a particular geodesic in the family, and t is the usual curve parameter, which can be taken to be time. (In this section, Latin indices are used in the description of the Riemannian manifold. Also, the x^j in equation 55 are not to be confused with the x_σ of sections 1 and 2.) The Riemannian geodesic equation in a coordinate representation is given by (*18*)

$$\frac{\partial^2 x^j}{\partial t^2} + \Gamma^j_{kl}(s)\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t} = 0, \tag{56}$$

in which the Levi-Civita connection is given by

$$\Gamma^j_{kl}(s) = \frac{1}{2} g^{jm}(s)(g_{km,l}(s) + g_{lm,k}(s) - g_{kl,m}(s)), \tag{57}$$

for metric $g_{ij}(x(s,t)) \equiv g_{ij}(s)$. (Partial derivatives are used in equation 56 to distinguish the s from the t dependence.) The geodesic equation, equation 59, on the $SU(2^n)$ group manifold can be shown to also follow from equation 56 (*1, 2*).

Let $x^j(0,t)$ be the base geodesic, and define the lifted Jacobi field along the base geodesic by (*1*)

$$J^j(t) = \frac{\partial}{\partial s} x^j(s,t)_{|s=0}, \tag{58}$$

describing how the base geodesic changes as the parameter s is varied. Using a Taylor series expansion, one has for small Δs in the neighborhood of the base geodesic,

$$x^j(\Delta s, t) = x^j(0,t) + \Delta s J^j(t) + O(\Delta s^2). \tag{59}$$

Here $x^j(\Delta s, t)$ satisfies the geodesic equation with the metric $g_{ij}(\Delta s)$. Operating on the geodesic equation, equation 56 with $\partial_s \equiv \frac{\partial}{\partial s}$ and substituting equations 58 and 59, one obtains for $\Delta s \to 0$,

$$\begin{aligned} 0 \;=\; & \frac{\partial^2}{\partial t^2} \operatorname*{Lim}_{\Delta s \to 0} \frac{\Delta s J^j(t)}{\Delta s} + \Gamma^j_{kl,m}(s)_{|s=0} \operatorname*{Lim}_{\Delta s \to 0} \frac{\Delta s J^m(t)}{\Delta s} \frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t} + \partial_s \Gamma^j_{kl}(s)_{|s=0} \frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t} \\ & + \Gamma^j_{kl}(0) \left\{ \frac{\partial}{\partial t}\left(\operatorname*{Lim}_{\Delta s \to 0} \frac{\Delta s J^k(t)}{\Delta s} \right) \frac{\partial x^l}{\partial t} + \frac{\partial x^k}{\partial t} \frac{\partial}{\partial t} \operatorname*{Lim}_{\Delta s \to 0} \frac{\Delta s J^l(t)}{\Delta s} \right\}, \end{aligned} \tag{60}$$

in which $g_{ij}(0) \equiv g_{ij}$ is the base metric and $\Gamma^j_{kl}(0) \equiv \Gamma^j_{kl}$ is the base connection. Equation 60 then becomes

$$\begin{aligned} 0 &= \frac{\partial^2 J^j(t)}{\partial t^2} + \Gamma^j_{kl,m}(s)_{|s=0} J^m(t) \frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t} \\ &+ \partial_s \Gamma^j_{kl}(s)_{|s=0} \frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t} + \Gamma^j_{kl}\left(\frac{\partial J^k}{\partial t}\frac{\partial x^l}{\partial t} + \frac{\partial x^k}{\partial t}\frac{\partial J^l}{\partial t}\right). \end{aligned} \tag{61}$$

Taking account of dummy indices summed over, it is clearly true that

$$-\Gamma^j_{lq}\Gamma^q_{ik}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k + \Gamma^j_{kp}\Gamma^p_{mn}\frac{\partial x^k}{\partial t}\frac{\partial x^m}{\partial t}J^n = 0. \tag{62}$$

One also has

$$-\Gamma^j_{ik,l}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k + \Gamma^j_{kp,m}\frac{\partial x^m}{\partial t}\frac{\partial x^k}{\partial t}J^p = 0. \tag{63}$$

Also, using the geodesic equation, equation 56, one has

$$\Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}J^p = -\Gamma^j_{kp}\Gamma^k_{iq}\frac{\partial x^i}{\partial t}\frac{\partial x^q}{\partial t}J^p, \tag{64}$$

or renaming dummy indices on the right hand side, it follows that

$$\Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}J^p + \Gamma^j_{qk}\Gamma^q_{il}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k = 0. \tag{65}$$

Next adding equations 61–63 and 65, one obtains

$$\begin{aligned} 0 &= \frac{\partial^2 J^j(t)}{\partial t^2} + \Gamma^j_{kl,m} J^m(t) \frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t} \\ &+ \partial_s \Gamma^j_{kl}(s)_{|s=0} \frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t} + \Gamma^j_{kl}\left(\frac{\partial J^k}{\partial t}\frac{\partial x^l}{\partial t} + \frac{\partial x^k}{\partial t}\frac{\partial J^l}{\partial t}\right) \\ &- \Gamma^j_{lq}\Gamma^q_{lk}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k + \Gamma^j_{kp}\Gamma^p_{mn}\frac{\partial x^k}{\partial t}\frac{\partial x^m}{\partial t}J^n \\ &- \Gamma^j_{ik,l}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k + \Gamma^j_{kp,m}\frac{\partial x^m}{\partial t}\frac{\partial x^k}{\partial t}J^p + \Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}J^p + \Gamma^j_{qk}\Gamma^q_{il}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k, \end{aligned} \tag{66}$$

or equivalently,

$$\begin{aligned} \frac{\partial^2 J^j(t)}{\partial t^2} &= -\Gamma^j_{kl,m}\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t}J^m + \Gamma^j_{lq}\Gamma^q_{ik}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k \\ &- \Gamma^j_{kp}\Gamma^p_{mn}\frac{\partial x^k}{\partial t}\frac{\partial x^m}{\partial t}J^n - \Gamma^j_{qk}\Gamma^q_{il}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k + \Gamma^j_{ik,l}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k - \Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}J^p \\ &- \Gamma^j_{kl}\left(\frac{\partial J^k}{\partial t}\frac{\partial x^l}{\partial t} + \frac{\partial x^k}{\partial t}\frac{\partial J^l}{\partial t}\right) - \partial_s \Gamma^j_{kl}(s)_{|s=0}\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t} - \Gamma^j_{kp,m}\frac{\partial x^m}{\partial t}\frac{\partial x^k}{\partial t}J^p. \end{aligned} \tag{67}$$

Rearranging terms in equation 67, then

$$\begin{aligned}
\frac{\partial^2 J^j(t)}{\partial t^2} &= \Gamma^j_{ik,l}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k - \Gamma^j_{kl,m}\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t}J^m + \Gamma^j_{lq}\Gamma^q_{ik}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k \\
&\quad -\Gamma^j_{kp}\Gamma^p_{mn}\frac{\partial x^k}{\partial t}\frac{\partial x^m}{\partial t}J^n - \Gamma^j_{kp,m}\frac{\partial x^m}{\partial t}\frac{\partial x^k}{\partial t}J^p - \Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}J^p \\
&\quad -\Gamma^j_{kl}\frac{\partial x^k}{\partial t}\frac{\partial J^l}{\partial t} - \Gamma^j_{kl}\frac{\partial x^l}{\partial t}\frac{\partial J^k}{\partial t} \\
&\quad -\Gamma^j_{qk}\Gamma^q_{il}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k - \partial_s\Gamma^j_{kl}(s)_{|s=0}\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t}.
\end{aligned} \tag{68}$$

Recalling that the Levi-Civita connection is symmetric, one has

$$\Gamma^j_{qp} = \Gamma^j_{pq}, \tag{69}$$

and renaming dummy indices, equation 68 becomes

$$\begin{aligned}
\frac{\partial^2 J^j}{\partial t^2} &= \left(\Gamma^j_{ik,l} - \Gamma^j_{il,k} + \Gamma^j_{lq}\Gamma^q_{ik} - \Gamma^j_{kp}\Gamma^p_{li}\right)\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k \\
&\quad -\Gamma^j_{kp,m}\frac{\partial x^m}{\partial t}\frac{\partial x^k}{\partial t}J^p - \Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}J^p - \Gamma^j_{kl}\frac{\partial x^k}{\partial t}\frac{\partial J^l}{\partial t} \\
&\quad -\Gamma^j_{pk}\frac{\partial x^k}{\partial t}\left(\frac{\partial J^p}{\partial t} + \Gamma^p_{mn}\frac{\partial x^m}{\partial t}J^n\right) - \partial_s\Gamma^j_{kl}(s)_{|s=0}\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t}.
\end{aligned} \tag{70}$$

Using the well-known expression for the covariant derivative (*22, 29*), it follows that

$$\begin{aligned}
\frac{D^2 J^j}{Dt^2} &= \frac{\partial}{\partial t}\left(\frac{DJ^j}{Dt}\right) + \Gamma^j_{kp}\frac{\partial x^k}{\partial t}\frac{DJ^p}{Dt} \\
&= \frac{\partial}{\partial t}\left(\frac{\partial J^j}{\partial t} + \Gamma^j_{kp}\frac{\partial x^k}{\partial t}J^p\right) + \Gamma^j_{kp}\frac{\partial x^k}{\partial t}\frac{DJ^p}{Dt},
\end{aligned} \tag{71}$$

or

$$\begin{aligned}
\frac{D^2 J^j}{Dt^2} &= \frac{\partial^2 J^j}{\partial t^2} + \Gamma^j_{kp,m}\frac{\partial x^m}{\partial t}\frac{\partial x^k}{\partial t}J^p + \Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}J^p + \Gamma^j_{kp}\frac{\partial x^k}{\partial t}\frac{\partial J^p}{\partial t} \\
&\quad +\Gamma^j_{kp}\frac{\partial x^k}{\partial t}\left(\frac{\partial J^p}{\partial t} + \Gamma^p_{mn}\frac{\partial x^m}{\partial t}J^n\right).
\end{aligned} \tag{72}$$

Next the well-known Riemann curvature tensor is given by (*29*)

$$R^j_{ikl} = \Gamma^j_{il,k} - \Gamma^j_{ik,l} + \Gamma^j_{kp}\Gamma^p_{li} - \Gamma^j_{lq}\Gamma^q_{ik}. \tag{73}$$

Substituting equations 79 and 73 in equation 72, one obtains the so-called lifted Jacobi equation (*1*):

$$\frac{D^2 J^j}{Dt^2} + R^j_{ikl}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k + \partial_s\Gamma^j_{kl}(s)_{|s=0}\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t} = 0. \tag{74}$$

This equation is useful for investigations of the global behavior of geodesics and their extrapolation to values of the parameter s characterizing neighboring geodesics on the Riemannian manifold (*1*).

If g_{ij} is independent of s, one has

$$\partial_s \Gamma^j_{kl}(s)_{|s=0} = 0; \tag{75}$$

the last term of equation 74 is then vanishing, and one obtains the standard Jacobi equation for the Jacobi vector J^j (*18*),

$$\frac{D^2 J^j}{Dt^2} + R^j_{ikl} \frac{\partial x^i}{\partial t} \frac{\partial x^l}{\partial t} J^k = 0. \tag{76}$$

Equation 76 is also known as the equation of geodesic deviation (*33, 29*), measuring the local convergence or divergence of neighboring geodesics, and it is useful in the determination of possible geodesic conjugate points (*18, 1*). (Again it is well to recall that conjugate points are points on a geodesic at which the Jacobi field is vanishing without vanishing in between those points. It is well-known that past the first conjugate point, a geodesic ceases to be minimizing (*15, 18*).

Next consider the factor in the last term of the lifted Jacobi equation, equation 74,

$$L^j_{kl} \equiv \partial_s \Gamma^j_{kl}(s)_{|s=0}. \tag{77}$$

Substituting equation 57 in equation 77, one has

$$L^j_{kl} \equiv \left\{ \partial_s \left[\frac{1}{2} g^{jm}(s)(g_{km,l}(s) + g_{lm,k}(s) - g_{kl,m}(s) \right] \right\}_{|s=0}, \tag{78}$$

or equivalently,

$$L^j_{kl} \equiv \frac{\partial g^{jm}(s)}{\partial s}_{|s=0} \Gamma_{mkl} + \frac{1}{2} g^{jm}(g'_{km,l} + g'_{lm,k} - g'_{kl,m}), \tag{79}$$

in which one defines

$$g'_{km} \equiv \partial_s g_{km}(s)_{|s=0}. \tag{80}$$

Using the well-known expression for the covariant derivative of a second rank tensor (*29*), one has

$$g'_{km;l} = g'_{km,l} - g'_{ki}\Gamma^i_{ml} - g'_{mi}\Gamma^i_{kl}. \tag{81}$$

Then substituting equation 81 in equation 79, one obtains

$$\begin{aligned} L^j_{kl} \equiv \frac{\partial g^{jm}(s)}{\partial s}_{|s=0} \Gamma_{mkl} + \frac{1}{2} g^{jm}(& g'_{km;l} + g'_{ki}\Gamma^i_{ml} + g'_{mi}\Gamma^i_{kl} \\ & + g'_{lm;k} + g'_{li}\Gamma^i_{mk} + g'_{mi}\Gamma^i_{kl} \\ & - g'_{kl;m} - g'_{ki}\Gamma^i_{lm} - g'_{li}\Gamma^i_{km}), \end{aligned} \tag{82}$$

and using equation 69, then

$$L^j_{kl} \equiv \frac{1}{2}g^{jm}(g'_{km;l} + g'_{lm;k} - g'_{kl;m}) + \frac{\partial g^{jm}(s)}{\partial s}_{|s=0}\Gamma_{mkl} + g^{jm}g'_{mi}\Gamma^i_{kl}. \tag{83}$$

Next noting that

$$(g^{jm}g_{mi})' = (\delta^j_i)' = 0, \tag{84}$$

then

$$g^{jm}(0)\left(\frac{\partial}{\partial s}g_{mi}(s)\right)_{|s=0} = -\left(\frac{\partial g^{jm}(s)}{\partial s}\right)_{|s=0} g_{mi}(0). \tag{85}$$

Multiplying both sides of equation 85 by Γ^i_{kl}, and using equation 80, one obtains

$$g^{jm}g'_{mi}\Gamma^i_{kl} = -\left(\frac{\partial g^{jm}(s)}{\partial s}\right)_{|s=0}\Gamma_{mkl}, \tag{86}$$

so that equation 83 reduces to

$$L^j_{kl} \equiv \frac{1}{2}g^{jm}(g'_{km;l} + g'_{lm;k} - g'_{kl;m}). \tag{87}$$

Finally then combining equations 74, 77, and 87, one obtains

$$\frac{D^2J^j}{Dt^2} + R^j_{ikl}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k + \frac{1}{2}g^{jm}(g'_{km;l} + g'_{lm;k} - g'_{kl;m})\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t}. \tag{88}$$

Next define the vector field,

$$C^j \equiv \frac{1}{2}g^{jm}(g'_{km;l} + g'_{lm;k} - g'_{kl;m})\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t}, \tag{89}$$

which is independent of the Jacobi field J^j. Equivalently, by symmetry, equation 89 can also be written as

$$C^j \equiv \frac{1}{2}g^{jm}(2g'_{km;l} - g'_{kl;m})\frac{\partial x^k}{\partial t}\frac{\partial x^l}{\partial t}. \tag{90}$$

Substituting equation 81 in equation 88, one obtains the second-order differential equation,

$$\frac{D^2J^j}{Dt^2} + R^j_{ikl}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}J^k + C^j = 0, \tag{91}$$

the so-called "lifted Jacobi equation" (*1*). Nielsen and Dowling used the lifted Jacobi equation, equation 91, adapted to the $SU(2^n)$ group manifold, to deform geodesics by varying the penalty parameter q (see section 4). This enabled them to define a so-called "geodesic derivative" and to numerically deform a geodesic as the penalty parameter q is varied without changing the fixed values $U = 1$ and $U = U_f$ of the initial and final unitary transformation corresponding to a quantum computation (*1*).

The generic lifted Jacobi equation, equation 91, can be solved. One first rewrites equation 72 as

$$\begin{aligned}\frac{D^2 J^j}{Dt^2} &= \frac{\partial^2 J^j}{\partial t^2} + 2\Gamma^j_{kp}\frac{\partial x^k}{\partial t}\frac{\partial J^p}{\partial t} + \Gamma^j_{kp,m}\frac{\partial x^m}{\partial t}\frac{\partial x^k}{\partial t}J^p + \Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}J^p \\ &\quad + \Gamma^j_{kp}\frac{\partial x^k}{\partial t}\Gamma^p_{mn}\frac{\partial x^m}{\partial t}J^n, \end{aligned} \tag{92}$$

and renaming dummy indices in the last term, then

$$\begin{aligned}\frac{D^2 J^j}{Dt^2} &= \frac{\partial^2 J^j}{\partial t^2} + \left(2\Gamma^j_{kp}\frac{\partial x^k}{\partial t}\right)\frac{\partial J^p}{\partial t} \\ &\quad + \left(\Gamma^j_{kp,m}\frac{\partial x^m}{\partial t}\frac{\partial x^k}{\partial t} + \Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2} + \Gamma^j_{kq}\frac{\partial x^k}{\partial t}\Gamma^q_{mp}\frac{\partial x^m}{\partial t}\right)J^p, \end{aligned} \tag{93}$$

or equivalently

$$\frac{D^2 J^j}{Dt^2} = \frac{\partial^2 J^j}{\partial t^2} + A^j_p\frac{\partial J^p}{\partial t} + \left(\sum_{n=1}^{3} {}^{(n)}B^j_p\right)J^p, \tag{94}$$

where

$$A^j_p \equiv \left(2\Gamma^j_{kp}\frac{\partial x^k}{\partial t}\right), \tag{95}$$

$${}^{(1)}B^j_p \equiv \Gamma^j_{kp,m}\frac{\partial x^m}{\partial t}\frac{\partial x^k}{\partial t}, \tag{96}$$

$${}^{(2)}B^j_p \equiv \Gamma^j_{kp}\frac{\partial^2 x^k}{\partial t^2}, \tag{97}$$

and

$${}^{(3)}B^j_p \equiv \Gamma^j_{kq}\frac{\partial x^k}{\partial t}\Gamma^q_{mp}\frac{\partial x^m}{\partial t}. \tag{98}$$

Next equation 91 can written as

$$\frac{D^2 J^j}{Dt^2} + {}^{(4)}B^j_p J^p + C^j = 0, \tag{99}$$

where

$${}^{(4)}B^j_p \equiv R^j_{ipl}\frac{\partial x^i}{\partial t}\frac{\partial x^l}{\partial t}. \tag{100}$$

Next substituting equation 99 in equation 94, one obtains

$$\frac{\partial^2 J^j}{\partial t^2} + A^j_p\frac{\partial J^p}{\partial t} + B^j_p J^p + C^j = 0, \tag{101}$$

where

$$B^j_p = \sum_{n=1}^{4} {}^{(n)}B^j_p. \tag{102}$$

Next define the column vectors

$$J \equiv \left[J^j\right], \tag{103}$$

$$C \equiv \left[C^j\right], \tag{104}$$

and the matrices

$$A \equiv \left[A_p^j\right], \tag{105}$$

$$B \equiv \left[B_p^j\right] = \left[\sum_{n=1}^{4} {}^{(n)}B_p^j.\right]. \tag{106}$$

Equation 101 then becomes

$$\frac{\partial^2 J}{\partial t^2} + A\frac{\partial J}{\partial t} + BJ + C = 0. \tag{107}$$

Furthermore, defining the column vector

$$K \equiv \left[\begin{array}{c} J_1 \\ J_2 \end{array}\right] \equiv \left[\begin{array}{c} J \\ \frac{\partial J}{\partial t} \end{array}\right], \tag{108}$$

then equation 107 is equivalent to

$$\frac{\partial K}{\partial t} \equiv \left[\begin{array}{cc} 0 & I \\ -B & -A \end{array}\right] K - \left[\begin{array}{c} 0 \\ C \end{array}\right]. \tag{109}$$

The homogeneous part of equation 109 with $C = 0$ is equivalent to the Jacobi equation, equation 76, and is given by

$$\frac{\partial K_0}{\partial t} \equiv MK_0, \tag{110}$$

in which the matrix M is given by

$$M \equiv \left[\begin{array}{cc} 0 & I \\ -B(t) & -A(t) \end{array}\right], \tag{111}$$

and the time dependence of A and B is indicated explicitly. The solution to the Jacobi equation, equation 110, is given in terms of the time-ordered exponential (*34, 25*), namely,

$$K_0(t) = \left(I + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^t dt_1 .. \int_0^t dt_n \mathrm{T}(M(t_1)...M(t_n))\right) K_0(0), \tag{112}$$

where T denotes the time ordering operator (not to be confused with the transpose of a matrix, appearing below). Thus, equation 112 gives the Jacobi field and can be expressed formally as

$$K_0(t) = \mathrm{T}\exp\left(\int_0^t dt' M(t')\right) K_0(0), \tag{113}$$

or defining the operator

$$E_t \equiv \mathrm{T}\exp\left(\int_0^t dt' M(t')\right) = I + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^t dt_1 .. \int_0^t dt_n \mathrm{T}(M(t_1)...M(t_n)). \tag{114}$$

Equation 113 can also be written as

$$K_0(t) = E_t K_0(0). \tag{115}$$

It follows from equation 114 that

$$\begin{aligned}
\frac{\partial E_t}{\partial t} &= M(t) + \sum_{n=2}^{\infty} \frac{1}{n!} n \int_0^t dt_1 .. \int_0^t dt_{n-1} \mathrm{T}(M(t_1)...M(t_{n-1})M(t)) \\
&= M(t) + M(t) \sum_{n=2}^{\infty} \frac{1}{(n-1)!} \int_0^t dt_1 .. \int_0^t dt_{n-1} \mathrm{T}(M(t_1)...M(t_{n-1})) \\
&= M(t) \left(I + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^t dt_1 .. \int_0^t dt_n \mathrm{T}(M(t_1)...M(t_n)) \right),
\end{aligned} \tag{116}$$

or equivalently then substituting equation 114, one obtains

$$\frac{\partial E_t}{\partial t} = M(t) E_t. \tag{117}$$

The solution to the inhomogeneous equation, equation 109 is given by

$$K(t) = E_t K(0) - E_t \int_0^t dr E_r^{-1} \begin{bmatrix} 0 \\ C(r) \end{bmatrix}. \tag{118}$$

This is the lifted Jacobi field. To see that equation 118 solves the inhomogeneous equation, equation 109, one notes that using equations 118 and 117 one has

$$\begin{aligned}
\frac{\partial K(t)}{\partial t} &= \frac{\partial E_t}{\partial t} K(0) - \frac{\partial E_t}{\partial t} \int_0^t dr E_r^{-1} \begin{bmatrix} 0 \\ C(r) \end{bmatrix} - E_t E_t^{-1} \begin{bmatrix} 0 \\ C(t) \end{bmatrix} \\
&= M(t) E_t K(0) - M(t) E_t \int_0^t dr E_r^{-1} \begin{bmatrix} 0 \\ C(r) \end{bmatrix} - \begin{bmatrix} 0 \\ C(t) \end{bmatrix}.
\end{aligned} \tag{119}$$

Next substituting equations 115, 118, and 111 in equation 119, then

$$\begin{aligned}
\frac{\partial K(t)}{\partial t} &= M(t) E_t K(0) + M(t) K(t) - M(t) E_t K(0) - \begin{bmatrix} 0 \\ C(t) \end{bmatrix} \\
&= \begin{bmatrix} 0 & I \\ -B(t) & -A(t) \end{bmatrix} K(t) - \begin{bmatrix} 0 \\ C(t) \end{bmatrix},
\end{aligned} \tag{120}$$

and thus equation 109 is, in fact, satisfied by equation 118.

The manifold of interest in the present work is the $SU(2^n)$ group manifold. For this case, consider a base geodesic with coordinates $\gamma^\sigma(q, t)$ on the $SU(2^n)$ group manifold with

penalty parameter q, and a neighboring geodesic with coordinates $\gamma^\sigma(q+\Delta,t)$ with penalty parameter $q+\Delta$. To first order in Δ, one has

$$\gamma^\sigma(q+\Delta,t) = \gamma^\sigma(q,t) + \Delta J^\sigma(t), \tag{121}$$

in which the Jacobi field coordinates $J^\sigma(t)$ are defined by

$$J^\sigma(t) = \frac{\partial\gamma^\sigma(q,t)}{\partial q}. \tag{122}$$

The Hamiltonian for a geodesic $\gamma(t)$ with penalty parameter q is given by

$$H_q = \frac{d\gamma}{dt}. \tag{123}$$

Then one has

$$\frac{dH_q}{dq} = \frac{d}{dq}\frac{d\gamma}{dt}, \tag{124}$$

or equivalently,

$$\frac{dH_q}{dq} = \frac{d}{dt}\frac{d\gamma}{dq}, \tag{125}$$

and substituting equation 122 in equation 125, then

$$\frac{dH_q}{dq} = \frac{dJ}{dt}, \tag{126}$$

in which the Jacobi field J is

$$J = J^\sigma\sigma. \tag{127}$$

The geodesic equation for the base geodesic with penalty parameter q is given by equation 53, namely,

$$\frac{dL}{dt} = i[L,H], \tag{128}$$

where the dual L is given by

$$L = G(H). \tag{129}$$

The geodesic equation for the nearby geodesic with penalty parameter $q+\Delta$ is

$$\frac{d\overline{L}}{dt} = i[\overline{L},\overline{H}], \tag{130}$$

where

$$\overline{L} = \overline{G}(\overline{H}), \tag{131}$$

and in accord with equation 17,

$$\overline{G} = P + (q+\Delta)Q = G + \Delta\frac{dG}{dq} \equiv G + \Delta G', \tag{132}$$

in which

$$G' \equiv \frac{dG}{dq} = Q. \tag{133}$$

Next letting $U(t)$ and $\overline{U}(t)$ denote the geodesics for penalty parameter q and $q + \Delta$, respectively, then for small Δ one expects

$$\overline{U} = Ue^{-i\Delta J}, \tag{134}$$

and it follows that to first order in Δ,

$$\begin{aligned} \frac{d\overline{U}}{dt} &= \frac{dU}{dt}e^{-i\Delta J} + U\frac{d}{dt}\left(1 - i\Delta J + 0(\Delta^2)\right) \\ &= \frac{dU}{dt}e^{-i\Delta J} + U(-i\Delta\frac{dJ}{dt} + 0(\Delta^2)) \\ &= \frac{dU}{dt}e^{-i\Delta J} - iU\Delta\frac{dJ}{dt}. \end{aligned} \tag{135}$$

But according to the Schrődinger equation, one has

$$\frac{d\overline{U}}{dt} = -i\overline{HU} \tag{136}$$

and

$$\frac{dU}{dt} = -iHU, \tag{137}$$

so substituting equations 136 and 137 in equation 135, one obtains

$$-i\overline{HU} = -iHUe^{-i\Delta J} - iU\Delta\frac{dJ}{dt}, \tag{138}$$

or substituting equation 134, then equation 138 for small Δ becomes

$$-i\overline{H}Ue^{-i\Delta J} = -iHUe^{-i\Delta J} - iU\Delta\frac{dJ}{dt}, \tag{139}$$

or equivalently, then to order Δ,

$$-i\overline{H}U = -iHU - iU\Delta\frac{dJ}{dt}e^{i\Delta J} = -iHU - iU\Delta\frac{dJ}{dt}. \tag{140}$$

Next multiplying equation 140 on the right by $U^\dagger$ and noting that unitarity requires

$$UU^\dagger = 1, \tag{141}$$

then equation 140 becomes

$$\overline{H} = H + \Delta U\frac{dJ}{dt}U^\dagger \tag{142}$$

to first order in Δ. Next substituting equation 131 in equation 130, one obtains

$$\frac{d}{dt}(\overline{G(\overline{H})}) = i[\overline{G(\overline{H}}, \overline{H}]. \tag{143}$$

Then substituting equations 132 and 142 in the left side of equation 143, the left side becomes

$$\frac{d}{dt}(\overline{G(\overline{H})}) = \frac{d}{dt}((G + \Delta G')(H + \Delta K)), \tag{144}$$

where

$$K \equiv U \frac{dJ}{dt} U^{\dagger}. \tag{145}$$

Equivalently, equation 144 to first order in Δ is

$$\frac{d}{dt}(\overline{G(\overline{H})}) = \frac{d}{dt} G(H) + \Delta \frac{d}{dt}(G'(H) + G(K)). \tag{146}$$

Next, using equations 132, 142, and 1.45, the right side of equation 143 becomes

$$i[\overline{G(\overline{H}}, \overline{H}] = i[(G + \Delta G')(H + \Delta K), H + \Delta K], \tag{147}$$

or equivalently to first order in Δ,

$$i[\overline{G(\overline{H}}, \overline{H}] = i[G(H), H] + \Delta(i[G(H), K] + i[G'(H), H] + i[G(K), H]). \tag{148}$$

In terms of the dual, equation 129, equation 148 becomes

$$i[\overline{G(\overline{H}}, \overline{H}] = i[L, H] + \Delta(i[L, K] + i[G'(H), H] + i[G(K), H]). \tag{149}$$

Next substituting equations 146, 129, and 149 in equation 143, one obtains

$$\frac{d}{dt} L + \Delta(G'(\frac{d}{dt} H) + G(\frac{d}{dt} K)) = i[L, H] + \Delta(i[L, K] + i[G'(H), H] + i[G(K), H]), \tag{150}$$

and further substituting equation 128 in equation 150, one concludes that

$$G'(\frac{d}{dt} H) + G(\frac{d}{dt} K)) = i[L, K] + i[G'(H), H] + i[G(K), H]. \tag{151}$$

Furthermore, multiplying equation 151 on the left by G^{-1}, one obtains

$$G^{-1} G'(\frac{d}{dt} H) + \frac{d}{dt} K = G^{-1}(i[L, K] + i[G'(H), H] + i[G(K), H]). \tag{152}$$

But according to equations 128, 129, and 18,

$$\frac{d}{dt} H = i G^{-1}[L, H] = i F([L, H]), \tag{153}$$

so that, using equation 18, one has

$$G^{-1} G'(\frac{d}{dt} H) = F G'(\frac{d}{dt} H) = i F G' F([L, H]). \tag{154}$$

Then substituting equations 154 and 18 in equation 152, one obtains

$$0 = i F G' F([L, H]) + \frac{d}{dt} K + \ F(i[K, L] + i[H, G'(H)] + i[H, G(K)]), \tag{155}$$

or

$$0 = \frac{d}{dt}K + \ F(i[K, L] + i[H, G(K)] + G'F(i[L, H]) + i[H, G'(H)]). \tag{156}$$

Equation 156 is the lifted Jacobi equation for penalty parameter varied from q to $q + \Delta$ (*1*). It is an inhomogeneous first order differential equation in K.

If $G' = 0$, equation 156 reduces effectively to the conventional Jacobi equation, assuming the form,

$$0 = \frac{d}{dt}K + \ F(i[K, L] + i[H, G(K)]). \tag{157}$$

Equation 157 can be rewritten as follows using equations 2, 17, and 18:

$$\frac{d}{dt}K = -iF([P(K) + Q(K), P(H) + qQ(H)] + [P(H) + Q(H), P(K) + qQ(K)]). \tag{158}$$

Expanding the commutators, then

$$\begin{aligned} \frac{d}{dt}K \quad = \quad & -iF([P(K), P(H)] + q[P(K), Q(H)] \\ & +[Q(K), P(H)] + q[Q(K), Q(H)] \\ & +[P(H), P(K)] + q[P(H), Q(K)] \\ & +[Q(H), P(K)] + q[Q(H), Q(K)]). \end{aligned} \tag{159}$$

The first and fifth terms cancel, and also the forth and eighth terms cancel, so one obtains

$$\frac{d}{dt}K = -i(q-1)F([P(K), Q(H)] - [Q(K), P(H)]), \tag{160}$$

or equivalently,

$$\frac{d}{dt}K = -i(q-1)F([P(K), Q(H)] + [P(H), Q(K)]), \tag{161}$$

or

$$\frac{d}{dt}K = i(q-1)F([Q(H), P(K)] - [P(H), Q(K)]). \tag{162}$$

Solving equation 162 for K yields the conventional Jacobi field.

The inhomogeneous term in equation 156 is given by

$$C = F(G'F(i[L, H]) + i[H, G'(H)]). \tag{163}$$

Substituting equations 133, 49, 17, and 2 in equation 163, one has

$$\begin{aligned} C \quad &= \quad FQFi[(P + qQ)(H), P(H) + Q(H)] + Fi[H, Q(H)] \\ &= \quad FQFi\,([P(H), Q(H)] + q[Q(H), P(H)]) + Fi\,([P(H) + Q(H), Q(H)]) \\ &= \quad FQFi(1-q)[P(H), Q(H)] + Fi[P(H), Q(H)]. \end{aligned} \tag{164}$$

Equation 164 can be rewritten as follows:

$$\begin{aligned} C &= F(P+Q)Fi(1-q)[P(H),Q(H)] + Fi[P(H),Q(H)] \\ &\quad -FPFi(1-q)[P(H),Q(H)]. \end{aligned} \tag{165}$$

But using equations 2 and 18 one has

$$PF = P(P+\frac{1}{q}Q) = P^2 = P, \tag{166}$$

and using equations 2, 17, and 18, then equation 165 becomes

$$\begin{aligned} C &= F^2((1-q+F^{-1})i[P(H),Q(H)] - F^{-1}Pi(1-q)[P(H),Q(H)]) \\ &= F^2(1-q+P+qQ-P(1-q))i[P(H),Q(H)] \\ &= F^2(1-q+q(P+Q))i[P(H),Q(H)], \end{aligned} \tag{167}$$

or using equation 2, then

$$C = F^2 i[P(H),Q(H)]. \tag{168}$$

This is a useful form for the inhomogeneous term in the lifted Jacobi equation, equation 156 (*1*).

Next combining equations 156, 163, and 168, the lifted Jacobi equation for varying penalty parameter q is then given by

$$\frac{d}{dt}K = i(q-1)F([Q(H),P(K)] - [P(H),Q(K)]) - F^2 i[P(H),Q(H)]. \tag{169}$$

In terms of the solution for $K(t)$, the lifted Jacobi field for varying penalty parameter can first be written as

$$J(t) = J(0) + \int_0^t dt' \frac{dJ(t')}{dt'}. \tag{170}$$

But according to equations 145 and 141, one has

$$\frac{dJ(t)}{dt} = U^\dagger(t)K(t)U(t), \tag{171}$$

and substituting equation 171 in equation 170, one obtains

$$J(t) = J(0) + \int_0^t dt' U^\dagger(t')K(t')U(t'). \tag{172}$$

Next consider the case in which the Hamiltonian is constant along a geodesic. The geodesic equation 52 then implies

$$[G(H),H] = 0. \tag{173}$$

Also, using equations 54, 18, 2, 49, and 133, one has

$$
\begin{aligned}
0 &= \frac{dH}{dt} = G^{-1}\frac{dL}{dt} = iF[L, F(L)] = iF[L, P(L) + q^{-1}Q(L)] \\
&= iF[L, P(L) + q^{-1}(1-P)(L))] \\
&= i(1-q^{-1})F[L, P(L)] \\
&= i(1-q^{-1})F[P(H) + qQ(H), P(P(H) + qQ(H)] \\
&= i(1-q^{-1})F[P(H) + qQ(H), P(H)] \\
&= i(q-1)F[Q(H), P(H)] = i(1-q)F[P(H), Q(H)] \\
&= i(1-q)F[H, Q(H)] \\
&= i(1-q)F[H, G'(H)] = 0. \qquad (174)
\end{aligned}
$$

It then follows from equations 156, 173, and 174 that if the Hamiltonian is constant, then again one obtains the conventional Jacobi equation, equation 157. Thus if the Hamiltonian is constant, and $J(0) = 0$ and $dJ(0)/dt = 0$, then in accordance with equation 206 below, $J(t)$ is proportional to $dJ(0)/dt$ and therefore $J(t) = 0$. In this case, it then follows that the geodesics for the lifted Jacobi equation for varying penalty parameter remain the same as for the conventional Jacobi equation and are the same for all values of the penalty parameter q.

The so-called geodesic derivative can be used to determine geodesics that evolve from the identity to a chosen unitary transformation U (*1*). In quantum computation, one generally wishes the quantum computation to evolve to some final unitary transformataion which solves a given problem. One first chooses a Hamiltonian $H(0)$, which produces $U = \exp(-iH(0)T$ at some fixed time T along the geodesic for penalty parameter $q = 1$. The parameter q can next be varied to produce a corresponding change in the initial Hamiltonian, and this produces the so-called geodesic derivative $dH_q(0)/dq$. Integration then may produce a geodesic connecting the identity $U(0) = I$ and the chosen unitary transformation $U(T)$ for any penalty parameter q.

To proceed then, the general lifted Jacobi equation, equation 156, for varied penalty parameter can be solved. (It is convenient to solve equation 156 directly, instead of equation 169.) First substituting equation 103 in equation 156, one has

$$\frac{d}{dt}K = -i\ F([K, L] + [H, G(K)]) - C. \qquad (175)$$

The corresponding homogeneous equation is then

$$\frac{d}{dt}K_s = -i\ F([K_s, L] + [H, G(K_s)]), \qquad (176)$$

and it can be solved if it is first recast in vectorized form (*36, 37*). For any matrix

$$M = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{21} & \dots & a_{2n} \\ \vdots & \vdots & \dots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix}, \tag{177}$$

one defines the vectorized form of the matrix M by the column vector,

$$\text{vec } M = [a_{11}..a_{m1}, a_{12}..a_{m2}...a_{1n}...a_{mn}]^{\mathrm{T}}, \tag{178}$$

with each column of the matrix M appearing beneath the previous one, arranged in a column vector. If one has a matrix equation

$$C = AX + XB \tag{179}$$

for matrices A, B, C, and X, then it can be shown that (*36*)

$$\text{vec } C = \left[(I \otimes A) + (B^{\mathrm{T}} \otimes I)\right] \text{vec } X. \tag{180}$$

It then follows that the homogeneous equation 176 can be written in vectorized form as follows:

$$\begin{aligned} \frac{d}{dt}(\text{vec } K_s) &= -i\mathrm{F}\text{vec } [K_s L - L K_s + H G(K_s) - G(K_s) H] \\ &= i\mathrm{F}\text{vec } [(L K_s + K_s(-L)) - (H G(K_s) + G(K_s)(-H))] \\ &= i\mathrm{F}[(I \otimes L - L^{\mathrm{T}} \otimes I)\text{vec } K_s - (I \otimes H - H^{\mathrm{T}} \otimes I)\text{vec } \mathrm{G}(K_s)] \\ &= i\mathrm{F}[(I \otimes L - L^{\mathrm{T}} \otimes I) + (H^{\mathrm{T}} \otimes I - I \otimes H)\mathrm{G}]\text{vec } (K_s)] \\ &= iA\text{vec } K_s, \end{aligned} \tag{181}$$

where

$$A = \mathrm{F}\left[(I \otimes L - L^{\mathrm{T}} \otimes I) + (H^{\mathrm{T}} \otimes I - I \otimes H)\mathrm{G}\right], \tag{182}$$

and F and G are the vectorized forms of the superoperators F and G, respectively (*1*). For example, the superoperator F acting on the matrix X can clearly be written as

$$F(X) = \sum_j A_j X B_j, \tag{183}$$

for some matrices A_j and B_j. But one has (*36*)

$$\text{vec } A_j X B_j = (B_j^{\mathrm{T}} \otimes A_j)\text{vec } X, \tag{184}$$

and using equation 184 in equation 183, then

$$\text{vec } F(X) = \sum_j (B_j^{\mathrm{T}} \otimes A_j)\text{vec } X, \tag{185}$$

and therefore the vectorized form F of the superoperator F is given by

$$\mathrm{F} = \sum_j (B_j^{\mathrm{T}} \otimes A_j)\mathrm{vec}. \tag{186}$$

Evidently the solution to equation 181 is

$$\mathrm{vec}\ K_s(t) = \mathrm{T}\left(\exp\left(i\int_0^t A(t')dt'\right)\right)\mathrm{vec}\ K_s(0), \tag{187}$$

or

$$\mathrm{vec} K_s(t) = \kappa_t \mathrm{vec}\ K_s(0), \tag{188}$$

where

$$\kappa_t = \mathrm{T}\left(\exp\left(i\int_0^t A(t')dt'\right)\right). \tag{189}$$

It follows from equation 189 that

$$\frac{d}{dt}\kappa_t = iA(t)\kappa_t. \tag{190}$$

Here κ_t is the propagator for the homogeneous form of equation 175, namely, equation 176. The solution to equation 175 is then given by

$$K(t) = \mathrm{unvec}\left(\kappa_t \mathrm{vec}\ K(0) - \kappa_t \int_0^t dr \kappa_r^{-1} \mathrm{vec}\ C(r)\right), \tag{191}$$

in which unvec unvectorizes (*1*), namely, for a matrix M,

$$\mathrm{unvec}\ (\mathrm{vec}\ M) = M. \tag{192}$$

To see that equation 191 solves equation 175, one has

$$\frac{d}{dt}K(t) = \mathrm{unvec}\left(\frac{d}{dt}\kappa_t \mathrm{vec}\ K(0) - (\frac{d}{dt}\kappa_t)\int_0^t dr\kappa_r^{-1}\mathrm{vec}\ C(r) - \kappa_t\kappa_t^{-1}\mathrm{vec}\ C(t)\right). \tag{193}$$

Substituting equation 130 in equation 193, then

$$\frac{d}{dt}K(t) = \mathrm{unvec}\left(iA(t)\kappa_t \mathrm{vec}\ K(0) - iA(t)\kappa_t \int_0^t dr\kappa_t^{-1}\mathrm{vec}\ C(r) - \mathrm{vec}\ C(t)\right), \tag{194}$$

and substituting equation 193 in equation 194, then

$$\frac{d}{dt}K(t) = \mathrm{unvec}\left(iA(t)\kappa_t \mathrm{vec}\ K(0) + iA(t)(\mathrm{vec}\ K(t) - \kappa_t \mathrm{vec}\ K(0)) - \mathrm{vec}\ C(t)\right), \tag{195}$$

or

$$\frac{d}{dt}K(t) = \text{unvec}\left(iA(t)\text{vec } K(t) - \text{vec } C(t)\right). \tag{196}$$

Substituting equation 182 in equation 196, then

$$\frac{d}{dt}K(t) = \text{unvec}\big(i\text{F}\left[(I \otimes L - L^{\text{T}} \otimes I) + (H^{\text{T}} \otimes I - I \otimes H)\text{G}\right] \text{vec}K(t)\big) - C(t). \tag{197}$$

But according to equations 176, 181, and 182,

$$\text{unvec}\big(i\text{F}\left[(I \otimes L - L^{\text{T}} \otimes I) + (H^{\text{T}} \otimes I - I \otimes H)\text{G}\right] \text{vec}K(t)\big) = -i\ F([K, L] + [H, G(K)], \tag{198}$$

and then substituting equation 198 in equation 197 one obtains equation 175

$$\frac{d}{dt}K = -i\ F([K, L] + [H, G(K)] - C, \tag{199}$$

as required.

Next, in order to obtain the propagator of the standard (unlifted) Jacobi field J_s, using equation 184, then equation 171 in vectorized form is

$$\text{vec } (\frac{d}{dt}J_s) = (U^{\text{T}} \otimes U^{\dagger})\text{vec } K_s. \tag{200}$$

Substituting equation 188 in equation 200, then

$$\text{vec } (\frac{d}{dt}J_s) = (U^{\text{T}} \otimes U^{\dagger})\kappa_t\text{vec } K_s(0). \tag{201}$$

Next substituting equation 171 in equation 201,

$$\text{vec } (\frac{d}{dt}J_s) = (U^{\text{T}} \otimes U^{\dagger})\kappa_t\text{vec } (U(0)\frac{d}{dt}J_s(0)U(0)^{\dagger}), \tag{202}$$

then for $U(0) = I$, one has

$$\text{vec } (\frac{d}{dt}J_s) = (U^{\text{T}} \otimes U^{\dagger})\kappa_t\text{vec}\frac{d}{dt}J_s(0)). \tag{203}$$

Unvectorizing equation 203, then

$$\frac{d}{dt}J_s = \text{unvec } [(U^{\text{T}} \otimes U^{\dagger})\kappa_t(\text{vec}\frac{d}{dt}J_s(0))]. \tag{204}$$

But assuming $J_s(0) = 0$, one has

$$J_s(t) = \int_0^t dt'\frac{d}{dt}J_s(t'), \tag{205}$$

and substituting equation 204 in equation 205, then

$$J_s(t) = \int_0^t dt' \text{unvec } [(U^{\mathrm{T}} \otimes U^{\dagger})\kappa_{t'}(\text{vec } \frac{d}{dt'} J_s(0))]. \tag{206}$$

Next defining the propagator j_T that generates the standard unlifted Jacobi field at time T by

$$J_s(T) = j_T(\frac{d}{dt'} J_s(0)), \tag{207}$$

then according to equation 206, one has

$$j_T = \int_0^T dt' \text{unvec } (U^{\mathrm{T}} \otimes U^{\dagger})\kappa_{t'} \text{vec}. \tag{208}$$

It follows from equations 191, 171, 205 and the homogeneous term having the same form as equation 207 that at time T the solution to the lifted Jacobi equation for varying penalty parameter is given by

$$J(T) = j_T(\frac{d}{dt} J(0)) - \int_0^T dt U(t)^{\dagger} \left(\text{unvec } \kappa_t \left(\int_0^t dr \kappa_r^{-1} \text{vec } C(r) \right) \right) U(t). \tag{209}$$

If $J(T) = 0$ in equation 209, then

$$\frac{d}{dt} J(0) = j_T^{-1} \left[\int_0^T dt U(t)^{\dagger} \left(\text{unvec } \kappa_t \left(\int_0^t dr \kappa_r^{-1} \text{vec } C(r) \right) \right) U(t) \right]. \tag{210}$$

Next, according to equation 126, the Hamiltonian H_q for penalty parameter q is such that

$$\frac{d}{dq} H_q(0) = \frac{d}{dt} J(0), \tag{211}$$

and substituting equation 210 in equation 211, one obtains the so-called geodesic derivative (*1*)

$$\frac{d}{dq} H_q(0) = j_T^{-1} \left[\int_0^T dt U(t)^{\dagger} \text{unvec} \left(\kappa_t \left(\int_0^t dr \kappa_r^{-1} \text{vec } C(r) \right) \right) U(t) \right]. \tag{212}$$

For $q = 1$, one has, according to equations 2, 17, and 18,

$$F = P + \frac{1}{q} Q = P + Q = G = 1, \qquad q = 1, \tag{213}$$

and then according to equation 48 the Hamiltonian is constant,

$$\frac{dH}{dt} = 0, \qquad q = 1. \tag{214}$$

Then equation 168 becomes

$$C = i[P(H), Q(H)], \quad q = 1, \tag{215}$$

and then because of equation 214,

$$\frac{dC}{dt} = 0, \quad q = 1. \tag{216}$$

Therefore in equation 212 for $q = 1$ one has using equations 68 and 213,

$$Z \equiv \kappa_t \left(\int_0^t dr \kappa_r^{-1} \mathrm{vec}\ C(r) \right) = \kappa_t \left(\int_0^t dr \kappa_r^{-1} i\mathrm{vec}\ [P(H), Q(H)] \right), \tag{217}$$

and therefore

$$\frac{dZ}{dt} \equiv \left[\frac{d\kappa_t}{dt} \left(\int_0^t dr \kappa_r^{-1} \right) + 1 \right] i\mathrm{vec}\ [P(H), Q(H)]. \tag{218}$$

But for $q = 1$ in equation 182, one has, according to equations 213, 17, and 49, $F = 1$, $G = 1$, and $L = H$, and therefore

$$A = [I \otimes H - H^{\mathrm{T}} \otimes I + H^{\mathrm{T}} \otimes I - I \otimes H] = 0, \quad q = 1. \tag{219}$$

Then substituting equation 219 in equation 190, one obtains

$$\frac{d\kappa_t}{dt} = 0. \tag{220}$$

Also, according to equation 189 for $t = 0$, one has

$$\kappa_t = 1. \tag{221}$$

Then substituting equation 220 in equation 218, one obtains

$$\frac{dZ}{dt} \equiv i\mathrm{vec}\ [P(H), Q(H)]. \tag{222}$$

Also, according to equations 217 and 221,

$$Z(0) = 0. \tag{223}$$

Then combining equations 222 and 223, one obtains for $q = 1$,

$$Z = it\mathrm{vec}\ [P(H), Q(H)], \quad q = 1, \tag{224}$$

or using equations 217 and 224, then

$$\kappa_t \left(\int_0^t dr \kappa_r^{-1} \mathrm{vec}\ C(r) \right) = it\mathrm{vec}\ [P(H), Q(H)], \quad q = 1. \tag{225}$$

Substituting equation 225 in equation 212, then for $q = 1$, one has

$$\frac{d}{dq}H_q(0) = j_T^{-1}\left[\int_0^T dtU(t)^\dagger it[P(H), Q(H)]U(t)\right], \qquad q = 1. \tag{226}$$

For $q \neq 1$, one has, substituting equation 168 in equation 212,

$$\frac{d}{dq}H_q(0) = j_T^{-1}\left[\int_0^T dtU(t)^\dagger \text{unvec}\left(\kappa_t\left(\int_0^t dr\kappa_r^{-1}\text{vec } F^2 i[P(H), Q(H)]\right)\right)U(t)\right], \qquad q \neq 1. \tag{227}$$

Equations 226 and 227 give the so-called geodesic derivative (*1*) which is useful in the numerical determination of optimal geodesics representing a particular quantum computation.

4. Other Work

1. Solutions to the geodesic equation were addressed, describing possible minimum complexity paths in the $SU(2^n)$ group manifold and representing the unitary evolution associated with a quantum computation (*7*).

2. A known obstruction to numerically solving the geodesic equation is the so-called Razborov-Rudich theorem (*1*). It is possible that the obstruction, if it occurs, can be circumvented by introducing and tweaking an additional parameter (other than q) in the Hamiltonian. This parameter could be one multiplying only two-body terms.

5. Conclusions

In this work on the Riemannian geometry of quantum computation, the Riemann curvature and geodesic equation were reviewed, and the Jacobi equation and the lifted Jacobi equation on the manifold of the $SU(2^n)$ group of n-qubit unitary operators with unit determinant were explicitly derived using the Lie algebra $su(2^n)$. The Riemann curvature is given by equation 44. The geodesic equation is given by equation 54. The generic Jacobi equation and its solution are given by equations 76 and 112, respectively. The generic lifted Jacobi equation is given by equation 91, and the solution is given by equation 118. The lifted Jacobi equation on the $SU(2^n)$ manifold, for a varying penalty parameter, is given by equations 156 or 169, respectively, and the solution is given by equations 191 and 168. Also, the geodesic derivative is given by equation 212. These equations are germane to investigations of the global characteristics of geodesic paths (*15, 18*) and minimal complexity quantum circuits (*1, 28, 2*).

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7. Transitions

1. This work will supplement the small U.S. Army Research Laboratory (ARL)/Sensors and Electron Devices Directorate (SEDD) Mission Program on Quantum Computing.

2. I initiated collaborative research with Dr. John Myers and Prof. Tai Tsun Wu of Harvard University.

3. I wrote 10 papers (references 2–11).

4. I presented a American Mathematical Society (AMS) Short Course lecture on this work at American Mathematical Society Meeting in Washington DC.

5. I gave nine invited talks at international meetings.

6. I periodically informed a classified government group of progress on this research.

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